

# Single-layer model of reflective nanostructures for magneto-ellipsometry data analysis

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**Abstract.** In this work we present the method of magneto-ellipsometry data analysis. Magneto-ellipsometry measurements are conducted in situ during nanostructures synthesis. Magnetic field is applied in configuration of magneto-optical transverse Kerr effect. Single-layer model of reflective nanostructures is in focus.

## 1. Introduction

Magneto-ellipsometry is considered as one of powerful reliable nondestructive methods for nanostructures synthesis control that is highly important for spintronics, electronics and nanotechnology. This technique combines ellipsometry and magneto-optical Kerr effect measurements. Magneto-ellipsometry has to be developed and in this work we report on magneto-ellipsometry measurements analysis for the case of single-layer nanostructures study. We have developed the approach that can be applied to investigation of reflective ferromagnetic/non-ferromagnetic nanostructures that are a subject of interest due to observed spin transport phenomena. We offer an algorithm that yields information about dielectric permittivity tensor of ferromagnetic layer [1], where diagonal tensor elements are responsible for refractive index and extinction coefficient, off-diagonal tensor elements are related to magneto-optical effects:

$$[\varepsilon] = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{21} & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix} = \begin{bmatrix} \varepsilon'_{11} - i\varepsilon''_{11} & -i(\varepsilon'_{12} - i\varepsilon''_{12})(Q_1 - iQ_2) & 0 \\ i(\varepsilon'_{12} - i\varepsilon''_{12})(Q_1 - iQ_2) & \varepsilon'_{11} - i\varepsilon''_{11} & 0 \\ 0 & 0 & \varepsilon'_{11} - i\varepsilon''_{11} \end{bmatrix}, \quad (1)$$

where  $\varepsilon$  is a complex permittivity of a medium ( $\varepsilon_{11} = \varepsilon_{22} \approx \varepsilon_{33}$ ,  $\varepsilon_{12} = -\varepsilon_{21}$ ), real parts are marked by ', imaginary by '',  $Q = Q_1 - iQ_2$  is a proportional to magnetization magneto-optical parameter. In the non-magnetic condition ( $Q=0$ ) the off-diagonal tensor elements vanish.

In the following, we describe the method of interpretation of the ellipsometric and magneto-ellipsometric measurements data from the in situ setup of a magneto-optical generalized ellipsometer, which is integrated into an ultra-high vacuum chamber with the electromagnet for magnetization reversal of the sample. The key idea of this approach and the case of the model of a homogeneous semi-infinite medium have been reported in [2] and at the 8<sup>th</sup> Joint European Magnetic Symposia (JEMS-2016) [3]. Here we repeat some of our basic ideas and present developed expressions for

experimental data processing for a single-layer model of reflective nanostructures in order to study their optical and magneto-optical properties. We consider the case of electromagnetic wave incidence from non-magnetic dielectric medium (characterized by the refraction index  $N_0$ ) onto ferromagnetic metal (the refraction index  $N_1$ ) on substrate (the refraction index  $N_2$ ). We set the magnetization vector to be z-axis directed, so that YX plane is a plane of incidence, YZ plane is a boundary plane. The transverse configuration is in focus because of the design features of high-vacuum chamber and electromagnet that are commonly used for magnetization reversal. In this paper, we consider the visible light range, as a great amount of modern ellipsometers work in this range.

## 2. Ellipsometry and magneto-ellipsometry measurements data

Let us denote the ellipsometric parameters in the non-magnetic condition ( $Q=0$ ) as  $\psi_0$  and  $\Delta_0$  [1]. In the case of magneto-ellipsometric characterization of the sample ( $Q=Q_1-iQ_2 \neq 0$ ) the surface transverse magneto-optical Kerr effect results in the ellipsometric angles corrections  $\delta\psi$  and  $\delta\Delta$ . Thus, the ellipsometric parameters become  $\psi_0+\delta\psi$ ,  $\Delta_0+\delta\Delta$ . It means that four independent real-valued quantities ( $\psi_0$ ,  $\delta\psi$ ,  $\Delta_0$ ,  $\delta\Delta$ ) are measured and, as a result, four real-valued quantities ( $\epsilon'_{11}$ ,  $\epsilon''_{11}$ ,  $\epsilon'_{12}$ ,  $\epsilon''_{12}$ ) can be derived.

To start analysis of magneto-ellipsometry experimental data ( $\psi$  and  $\Delta$ ) we have to write the real and imaginary parts of complex reflection coefficients in the basic equation of ellipsometry [4, 5]:

$$\rho = \tan(\psi_0 + \delta\psi) \exp(i(\Delta_0 + \delta\Delta)) = R_p R_S^{-1} = (R'_p - iR''_p)(R'_S - iR''_S)^{-1}, \quad (2)$$

where  $\rho$  is the complex ellipsometric parameter,  $R_p$  and  $R_s$  are complex reflection coefficients corresponding to in-plane p-polarization and out-of-plane s-polarization respectively, real parts again are marked by ', imaginary by ". According to mode conversion from the p to the s polarized channel we can write that

$$R_p = R_{pp} + R_{ps} = R'_{p0} + R'_{p1} - i(R''_{p0} + R''_{p1}), \quad (3)$$

$$R_S = R_{SS} + R_{sp} = R'_{S0} - iR''_{S0}, \quad (4)$$

where we have distinguished the magnetic field contribution and marked it by subscript 1, non-magnetic summands – by subscript 0. One can see that transverse Kerr effect yields to  $R'_{sl}=0$ ,  $R''_{sl}=0$ .

By substituting equations (3-4) into (2) we obtain for non-magnetic condition:

$$\tan\psi_0 = \sqrt{\frac{(R'_{p0}R'_{S0} + R''_{S0}R''_{p0})^2 + (R''_{S0}R'_{p0} - R'_{p0}R''_{S0})^2}{R'^2_{S0} + R''^2_{S0}}}, \quad (5)$$

$$\Delta_0 = \arctg \frac{R''_{S0}R'_{p0} - R'_{p0}R''_{S0}}{R'_{p0}R'_{S0} + R''_{p0}R''_{S0}}, \quad (6)$$

while the influence of an external magnetic field leads to ellipsometric parameters  $\delta\psi$  and  $\delta\Delta$ :

$$\delta\psi = \psi - \psi_0 = \arctg(F \tan(\psi_0)) - \psi_0, \quad (7)$$

$$\delta\Delta = \Delta - \Delta_0 = \arctg \frac{R'_{S0}(R'_{p0} + R'_{p1}) - (R''_{p0} + R''_{p1})R'_{S0}}{(R'_{p0} + R'_{p1})R'_{S0} + (R''_{p0} + R''_{p1})R''_{S0}} - \arctg \frac{R'_{S0}R'_{p0} - R'_{p0}R''_{S0}}{R'_{p0}R'_{S0} + R''_{p0}R''_{S0}}, \quad (8)$$

where  $F$  is a helpful notation:

$$\tan(\psi_0 + \delta\psi) = F \tan(\psi_0) = \tan(\psi_0) \times \sqrt{1 + \frac{(R'_{S0}R'_{p1})^2 + (R'_{p1}R'_{S0})^2 + 2R'_{p0}R'_{p1}(R'^2_{S0} + R''^2_{S0})}{(R'_{p0}R'_{S0} + R''_{p0}R''_{S0})^2 + (R''_{S0}R'_{p0} - R'_{p0}R''_{S0})^2} + \frac{(R'_{p1}R'_{S0})^2 + (R'_{p1}R''_{S0})^2 + 2R'_{p0}R'_{p1}(R'^2_{S0} + R''^2_{S0})}{(R'_{p0}R'_{S0} + R''_{p0}R''_{S0})^2 + (R''_{S0}R'_{p0} - R'_{p0}R''_{S0})^2}}. \quad (9)$$

## 3. Data analysis

In Figure 1 one can see a diagram of single-layer model, where 0 – ambient medium, 1 – ferromagnetic metal (d – thickness), 2 – substrate,  $\varphi_0$ ,  $\varphi_1$  and  $\varphi_2$  are the angles of incidence and refraction and related to each other by Snell's law.

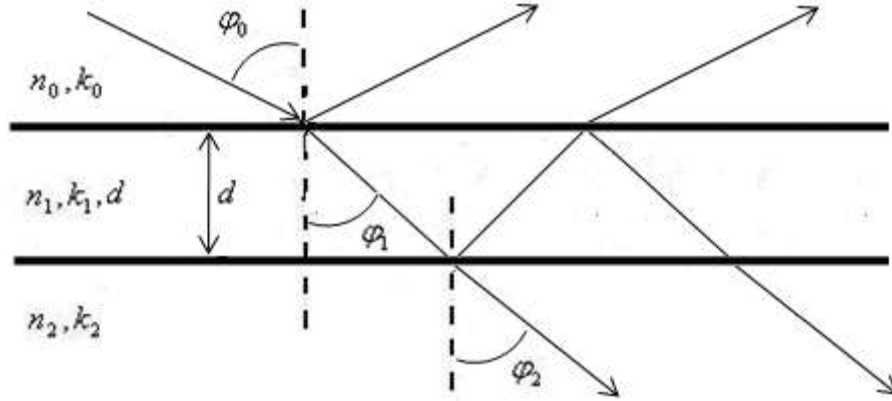


Figure 1 – Single-layer model of reflective nanostructures

For a single-layer model complex refractive indices of the material under study ( $N_1=n_1-ik_1$ ) are calculated from  $\psi_0, \Delta_0$  measurements by the Nelder-Mead method. The values of  $N_0=n_0-ik_0$ ,  $N_1=n_1-ik_1$ ,  $N_2=n_2-ik_2$  are necessary for the following ellipsometric angles calculation.

Analytical expressions for the Fresnel coefficients that take into account the magneto-optical parameter in the off-diagonal permittivity tensor elements were presented in [2, 4]. It was shown that the following expressions should be used for a single-layer model:

$$R_p = r_{01p} + \frac{t_{01p}t_{10p}r_{12p} \exp(-i2\beta)}{1 - r_{10p}r_{12p} \exp(-i2\beta)}, \quad (10)$$

$$R_s = \frac{r_{01s} + r_{12s} \exp(-i2\beta)}{1 + r_{01s}r_{12s} \exp(-i2\beta)}, \quad (11)$$

$$r_{01p} = \frac{N_1 \cos \varphi_0 - N_0 \cos \varphi_1}{N_1 \cos \varphi_0 + N_0 \cos \varphi_1} - i \frac{2QN^2_0 \sin \varphi_0 \cos \varphi_0}{(N_1 \cos \varphi_0 + N_0 \cos \varphi_1)^2}, \quad (12)$$

$$r_{12p} = \frac{N_2 \cos \varphi_1 - N_1 \cos \varphi_2}{N_2 \cos \varphi_1 + N_1 \cos \varphi_2} - i \frac{2QN^2_1 \sin \varphi_1 \cos \varphi_1}{(N_2 \cos \varphi_1 + N_1 \cos \varphi_2)^2}, \quad (13)$$

$$r_{10p} = \frac{N_0 \cos \varphi_1 - N_1 \cos \varphi_0}{N_0 \cos \varphi_1 + N_1 \cos \varphi_0} + i \frac{2QN^2_1 \sin \varphi_1 \cos \varphi_1}{(N_0 \cos \varphi_1 + N_1 \cos \varphi_0)^2}, \quad (14)$$

$$r_{01s} = \frac{N_0 \cos \varphi_0 - N_1 \cos \varphi_1}{N_0 \cos \varphi_0 + N_1 \cos \varphi_1}, \quad (15)$$

$$r_{12s} = \frac{N_1 \cos \varphi_1 - N_2 \cos \varphi_2}{N_1 \cos \varphi_1 + N_2 \cos \varphi_2}, \quad (16)$$

$$t_{01p} = \frac{2N_0 \cos \varphi_0}{N_1 \cos \varphi_0 + N_0 \cos \varphi_1} + i \frac{2QN^3_0 \sin \varphi_0 \cos \varphi_0}{N_1(N_1 \cos \varphi_0 + N_0 \cos \varphi_1)^2}, \quad (17)$$

$$t_{10p} = \frac{2N_1 \cos \varphi_1}{N_1 \cos \varphi_0 + N_0 \cos \varphi_1} - i \frac{2QN^3_1 \sin \varphi_1 \cos \varphi_1}{N_0(N_1 \cos \varphi_0 + N_0 \cos \varphi_1)^2}, \quad (18)$$

$$\beta_1 = \frac{2\pi}{\lambda} N_1 \cos \varphi_1 d_1, \quad (19)$$

where  $\beta_1$  is phase thickness of the film. Indices  $r_{01p}$ ,  $r_{01s}$  and  $r_{12p}$ ,  $r_{12s}$  in expressions (12, 15) and (13, 16) are the refractive indices for interfaces 0-1 and 1-2, respectively. Indices  $t_{01p}$  and  $t_{10p}$  in expressions (17, 18) are transmission coefficients. Indices  $r_{01p}$  and  $t_{01p}$  correspond to the wave propagation from

medium 0 to medium 1, while  $r_{10p}$  and  $t_{10p}$  – to the backward propagation. Taking into account expressions (3, 4) let us write  $r_{01p}$ ,  $r_{12p}$ ,  $r_{01s}$ ,  $r_{12s}$ ,  $r_{10p}$ ,  $t_{01p}$ ,  $t_{10p}$  in the same manner as the refractive indices and transmission coefficients for the model of a homogeneous semi-infinite medium:

$$r_{01s} = (R'_{s0})_{01} - i(R''_{s0})_{01}. \quad (20)$$

$$r_{12s} = (R'_{s0})_{12} - i(R''_{s0})_{12}. \quad (21)$$

$$r_{01p} = (R'_{p0})_{01} + (R'_{p1})_{01} - i((R''_{p0})_{01} + (R''_{p1})_{01}) = rr_{01} - i ri_{01}, \quad (22)$$

$$r_{12p} = (R'_{p0})_{12} + (R'_{p1})_{12} - i((R''_{p0})_{12} + (R''_{p1})_{12}) = rr_{12} - i ri_{12}, \quad (23)$$

$$r_{10p} = (R'_{p0})_{10} + (R'_{p1})_{10} - i((R''_{p0})_{10} + (R''_{p1})_{10}) = rr_{10} - i ri_{10}, \quad (24)$$

$$t_{01p} = (T'_{p0})_{01} + (T'_{p1})_{01} - i((T''_{p0})_{01} + (T''_{p1})_{01}) = tr_{01} - i ti_{01}, \quad (25)$$

$$t_{10p} = (T'_{p0})_{10} + (T'_{p1})_{10} - i((T''_{p0})_{10} + (T''_{p1})_{10}) = tr_{10} - i ti_{10}, \quad (26)$$

where  $(R'_{s0})_{01}$ ,  $(R'_{s0})_{12}$ ,  $(R'_{p0})_{01}$ ,  $(R'_{p0})_{12}$ ,  $(R'_{p1})_{01}$ ,  $(R'_{p1})_{12}$  are  $R'_{s0}$ ,  $R'_{s0}$ ,  $R'_{p0}$ ,  $R'_{p0}$ ,  $R'_{p1}$ ,  $R'_{p1}$  in the model of a homogeneous semi-infinite medium, respectively. Subscript 01 denotes the electromagnetic wave incidence from ambient medium 0 onto layer 1. Indices  $(R'_{s0})_{12}$ ,  $(R'_{s0})_{12}$ ,  $(R'_{p0})_{12}$ ,  $(R'_{p0})_{12}$ ,  $(R'_{p1})_{12}$ ,  $(R'_{p1})_{12}$  are also calculated by formulae for the model of a homogeneous semi-infinite medium, the only difference is that subscript 12 denotes the electromagnetic wave incidence from layer 1 onto substrate 2 that leads to the following changes:  $\cos \varphi_0 \rightarrow \cos \varphi_1$ ,  $\cos \varphi_1 \rightarrow \cos \varphi_2$ ,  $\sin \varphi_0 \rightarrow \sin \varphi_1$ ,  $n_1 \rightarrow n_2$ ,  $n_0 \rightarrow n_1$ ,  $k_1 \rightarrow k_2$ ,  $k_0 \rightarrow k_1$ . Likewise, indices  $(R'_{p0})_{10}$ ,  $(R'_{p0})_{10}$ ,  $(R'_{p1})_{10}$ ,  $(R'_{p1})_{10}$  describe the electromagnetic wave propagation from layer 1 to medium 0:  $\cos \varphi_0 \leftarrow \cos \varphi_1$ ,  $\sin \varphi_0 \leftarrow \sin \varphi_1$ ,  $n_0 \leftarrow n_1$ ,  $k_0 \leftarrow k_1$ .

Transmission coefficients were not involved into algorithm of data processing for the model of a homogeneous semi-infinite medium. Therefore, we report on  $(T'_{p0})_{01}$ ,  $(T'_{p0})_{12}$ ,  $(T'_{p1})_{01}$ ,  $(T'_{p1})_{12}$  here:

$$(T'_{p0})_{01} = 2 \frac{(n_0 n_1 + k_0 k_1)(a^2 + c^2) + (n_0^2 + k_0^2)(ab + cd)}{A_3^2 + B_3^2}, \quad (27)$$

$$(T'_{p0})_{12} = 2 \frac{(n_0^2 + k_0^2)(ad - bc) + (n_1 k_0 - n_0 k_1)(a^2 + c^2)}{A_3^2 + B_3^2}, \quad (28)$$

$$(T'_{p1})_{01} = 2 \frac{Q_1(pq + rs) - Q_2(pr - sq)}{(n_1^2 + k_1^2)(A_3^2 + B_3^2)^2}, \quad (29)$$

$$(T'_{p1})_{12} = 2 \frac{Q_1(pr - sq) + Q_2(pq + rs)}{(n_1^2 + k_1^2)(A_3^2 + B_3^2)^2}, \quad (30)$$

where

$$A_3 = n_1 a + k_1 c + n_0 b + k_0 d, \quad (31)$$

$$B_3 = k_1 a - n_1 c + k_0 b - n_0 d, \quad (32)$$

$$p = N(3n_0^2 k_0 - k_0^3) + P(n_0^3 - 3n_0 k_0^2), \quad (33)$$

$$q = n_1(A_3^2 - B_3^2) - 2A_3 B_3 k_1, \quad (34)$$

$$r = k_1(B_3^2 - A_3^2) - 2A_3 B_3 n_1, \quad (35)$$

$$s = N(n_0^3 - 3n_0 k_0^2) - P(3n_0^2 k_0 - k_0^3), \quad (36)$$

$$a = \text{Re}(\cos \varphi_0), \quad (37)$$

$$b = \text{Re}(\cos \varphi_1), \quad (38)$$

$$c = \text{Im}(\cos \varphi_0), \quad (39)$$

$$d = \text{Im}(\cos \varphi_1), \quad (40)$$

$$N = \text{Re}(\sin \varphi_0) a - \text{Im}(\sin \varphi_0) c \quad (41)$$

$$P = -\text{Re}(\sin \varphi_0) c - \text{Im}(\sin \varphi_0) a \quad (42)$$

Coefficients  $(T'_{p0})_{10}$ ,  $(T'_{p0})_{10}$ ,  $(T'_{p1})_{10}$ ,  $(T'_{p1})_{10}$  correspond to the electromagnetic wave propagation from layer 1 to medium 0, that leads to the changes:  $\cos \varphi_0 \leftarrow \varepsilon \cos \varphi_1$ ,  $\sin \varphi_0 \leftarrow \sin \varphi_1$ ,  $n_0 \leftarrow n_1$ ,  $k_0 \leftarrow k_1$ .

Let us take into account  $N_0 = n_0 - ik_0$ ,  $N_1 = n_1 - ik_1$ ,  $N_2 = n_2 - ik_2$ ,  $Q = Q_1 - iQ_2$  and compare expressions (10, 11) with (2, 3). Thus we obtain expressions for  $R'_{p0}$ ,  $R''_{p0}$ ,  $R'_{p1}$ ,  $R''_{p1}$ ,  $R'_{s0}$  and  $R''_{s0}$ .

$$R'_{p0} = (((R'_{p0})_{01} + \xi_1 (R'_{p0})_{12} - \eta_1 (R'_{p0})_{12}) (1 + \xi_1 L_{0112} - \eta_1 M_{0112}) + ((R''_{p0})_{01} + \eta_1 (R'_{p0})_{12} + \xi_1 (R''_{p0})_{12}) (\xi_1 M_{0112} + \eta_1 L_{0112})) (1 + \xi_1 L_{0112} - \eta_1 M_{0112})^2 + (\xi_1 M_{0112} + \eta_1 L_{0112})^2)^{-1}, \quad (43)$$

$$R''_{p0} = (((R'_{p0})_{01} + \eta_1 (R'_{p0})_{12} + \xi_1 (R'_{p0})_{12}) (1 + \xi_1 L_{0112} - \eta_1 M_{0112}) - ((R'_{p0})_{01} + \xi_1 (R'_{p0})_{12} - \eta_1 (R'_{p0})_{12}) (\xi_1 M_{0112} + \eta_1 L_{0112})) (1 + \xi_1 L_{0112} - \eta_1 M_{0112})^2 + (\xi_1 M_{0112} + \eta_1 L_{0112})^2)^{-1}, \quad (44)$$

$$R'_{p1} = \frac{\Omega \chi - \Gamma \varpi}{\Omega^2 + \Gamma^2} - R'_{p0}, \quad (45)$$

$$R''_{p1} = \frac{\Omega \varpi + \Gamma \chi}{\Omega^2 + \Gamma^2} - R''_{p0}, \quad (46)$$

$$R'_{s0} = (((R'_{s0})_{01} + \xi_1 (R'_{s0})_{12} - \eta_1 (R'_{s0})_{12}) (1 + \xi_1 H_{0112} - \eta_1 J_{0112}) + ((R''_{s0})_{01} + \eta_1 (R'_{s0})_{12} + \xi_1 (R''_{s0})_{12}) (\xi_1 J_{0112} + \eta_1 H_{0112})) (1 + \xi_1 H_{0112} - \eta_1 J_{0112})^2 + (\xi_1 J_{0112} + \eta_1 H_{0112})^2)^{-1}, \quad (47)$$

$$R''_{s0} = (((R'_{s0})_{01} + \eta_1 (R'_{s0})_{12} + \xi_1 (R'_{s0})_{12}) (1 + \xi_1 H_{0112} - \eta_1 J_{0112}) - ((R'_{s0})_{01} + \xi_1 (R'_{s0})_{12} - \eta_1 (R'_{s0})_{12}) (\xi_1 J_{0112} + \eta_1 H_{0112})) (1 + \xi_1 H_{0112} - \eta_1 J_{0112})^2 + (\xi_1 J_{0112} + \eta_1 H_{0112})^2)^{-1}, \quad (48)$$

where the following notations are used:

$$L_{0112} = (R'_{p0})_{12} (R'_{p0})_{01} - (R''_{p0})_{12} (R''_{p0})_{01}, \quad (49)$$

$$M_{0112} = (R'_{p0})_{01} (R''_{p0})_{12} + (R'_{p0})_{12} (R''_{p0})_{01}, \quad (50)$$

$$\xi_1 = \text{Re}(\exp(-i2\beta_1)), \quad (51)$$

$$\eta_1 = -\text{Im}(\exp(-i2\beta_1)), \quad (52)$$

$$J_{0112} = (R'_{s0})_{01} (R'_{s0})_{12} + (R'_{s0})_{12} (R'_{s0})_{01}, \quad (53)$$

$$H_{0112} = (R'_{s0})_{01} (R'_{s0})_{12} - (R'_{s0})_{12} (R'_{s0})_{01}, \quad (54)$$

$$\Omega = 1 - \xi_1 (rr_{10} rr_{12} - ri_{10} ri_{12}) + \eta_1 (ri_{10} rr_{12} + rr_{10} ri_{12}), \quad (55)$$

$$\varpi = ri_{01} - (\xi_1 rr_{12} - \eta_1 ri_{12}) (ri_{01} rr_{10} + ri_{10} rr_{01} - \tau) - (\xi_1 ri_{12} + \eta_1 rr_{12}) (rr_{01} rr_{10} - ri_{01} ri_{10} - \theta), \quad (56)$$

$$\Gamma = \xi_1 (ri_{10} rr_{12} + rr_{10} ri_{12}) + \eta_1 (rr_{10} rr_{12} - ri_{10} ri_{12}), \quad (57)$$

$$\chi = rr_{01} - (\xi_1 rr_{12} - \eta_1 ri_{12}) (rr_{01} rr_{10} - ri_{01} ri_{10} - \theta) + (\xi_1 ri_{12} + \eta_1 rr_{12}) (ri_{01} rr_{10} + ri_{10} rr_{01} - \tau), \quad (58)$$

$$\theta = tr_{01} tr_{10} - ti_{01} ti_{10}, \quad (59)$$

$$\tau = ti_{01} tr_{10} + ti_{10} tr_{01}. \quad (60)$$

Thus, we have all formulae that are necessary for theoretical calculation of the ellipsometric angles (2-9) in case of a single-layer model. Final step is giving the best fit to the experimental data by the use of the wavelength-to-wavelength Nelder–Mead minimization of the ellipsometric angles. It yields the spectral dependences of real ( $Q_1$ ) and imaginary parts ( $Q_2$ ) of magneto-optical parameter  $Q$ . So, we have information about all elements of the dielectric permittivity tensor.

#### 4. Conclusion

To conclude, we have proposed an approach to studying single-layer nanomaterials by means of magneto-ellipsometry. The algorithm of experimental data analysis ( $\psi_0$ ,  $\Delta_0$ ,  $\psi_0 + \delta\psi$ ,  $\Delta_0 + \delta\Delta$ ) is presented. As a result, optical and magneto-optical properties can be easily and reliably characterized during synthesis.

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